* * * * * * * * *   Welcome to STN International   * * * * * * * * * *

NEWS   1   Web Page URLs for STN Seminar Schedule - N. America
NEWS   2   "Ask CAS" for self-help around the clock
NEWS   3   May 12   EXTEND option available in structure searching
NEWS   4   May 12   Polymer links for the POLYLINK command completed in REGISTRY
NEWS   5   May 27   New UPM (Update Code Maximum) field for more efficient patent
                      SDIs in CAplus
NEWS   6   May 27   CAplus super roles and document types searchable in REGISTRY
NEWS   7   Jun 28   Additional enzyme-catalyzed reactions added to CASREACT
NEWS   8   Jun 28   ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG,
                      and WATER from CSA now available on STN(R)
NEWS   9   Jul 12   BEILSTEIN enhanced with new display and select options,
                      resulting in a closer connection to BABS
NEWS 10   Jul 30   BEILSTEIN on STN workshop to be held August 24 in conjunction
                      with the 228th ACS National Meeting
NEWS 11   AUG 02   IFIPAT/IFIUDB/IFICDB reloaded with new search and display
                      fields
NEWS 12   AUG 02   CAplus and CA patent records enhanced with European and Japan
                      Patent Office Classifications
NEWS 13   AUG 02   STN User Update to be held August 22 in conjunction with the
                      228th ACS National Meeting
NEWS 14   AUG 02   The Analysis Edition of STN Express with Discover!
                      (Version 7.01 for Windows) now available
NEWS 15   AUG 04   Pricing for the Save Answers for SciFinder Wizard within
                      STN Express with Discover! will change September 1, 2004
NEWS 16   AUG 27   BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 17   AUG 27   BIOTECHABS/BIOTECHDS: Two new display fields added for legal
                      status data from INPADOC
NEWS 18   SEP 01   INPADOC: New family current-awareness alert (SDI) available
NEWS 19   SEP 01   New pricing for the Save Answers for SciFinder Wizard within
                      STN Express with Discover!
NEWS 20   SEP 01   New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS 21   SEP 14   STN Patent Forum to be held October 13, 2004, in Iselin, NJ

NEWS EXPRESS   JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT
                 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
                 AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS   STN Operating Hours Plus Help Desk Availability
NEWS INTER   General Internet Information
NEWS LOGIN   Welcome Banner and News Items
NEWS PHONE   Direct Dial and Telecommunication Network Access to STN
NEWS WWW   CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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   * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 20:09:24 ON 14 SEP 2004

=> file hcaplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                    ENTRY   SESSION

h   eb c   g cg b   cg   eb

FULL ESTIMATED COST   0.21   0.21

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FILE COVERS 1907 - 14 Sep 2004   VOL 141 ISS 12
FILE LAST UPDATED: 13 Sep 2004   (20040913/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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L1   1 125:114681/DN

=> sel rn
E1 THROUGH E75 ASSIGNED

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              4 112677-04-0/BI
              6 113094-81-8/BI
           2953 122-01-0/BI
          14081 124-40-3/BI
            385 14254-57-0/BI
             14 142992-99-2/BI
              5 148077-69-4/BI
              7 152459-75-1/BI
              4 152459-76-2/BI
              4 152459-77-3/BI
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h   eb c   g cg b   cg   eb

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=> file reg
COST IN U.S. DOLLARS                             SINCE FILE        TOTAL
                                                   ENTRY          SESSION
FULL ESTIMATED COST                                 2.44           2.65
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DICTIONARY FILE UPDATES: 13 SEP 2004   HIGHEST RN 744170-41-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more
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=> d scan
YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS' - CONTINUE? (Y)/N:n
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=> file hcaplus
COST IN U.S. DOLLARS                             SINCE FILE        TOTAL
                                                   ENTRY          SESSION
FULL ESTIMATED COST                                 0.42           3.07
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FILE COVERS 1907 - 14 Sep 2004 VOL 141 ISS 12
FILE LAST UPDATED: 13 Sep 2004 (20040913/ED)

h   eb c   g cg b   cg   eb

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=> sel rn
TOO MANY ANSWER NUMBERS SPECIFIED
No more than 50000 answers may be specified.
ENTER ANSWER NUMBER OR RANGE (1-):0
NUMBERS IN RANGE MUST BE GREATER THAN ZERO.
An answer number must be a positive number.
ENTER ANSWER NUMBER OR RANGE (1-):end

=>.d his

     (FILE 'HOME' ENTERED AT 20:09:24 ON 14 SEP 2004)

     FILE 'HCAPLUS' ENTERED AT 20:09:32 ON 14 SEP 2004
L1          1 S 125:114681/DN
              SEL RN
L2      58357 S E1-E75

     FILE 'REGISTRY' ENTERED AT 20:09:49 ON 14 SEP 2004

     FILE 'HCAPLUS' ENTERED AT 20:09:57 ON 14 SEP 2004

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h   eb c   g cg b   cg   eb

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=> file reg
COST IN U.S. DOLLARS                          SINCE FILE       TOTAL



h        eb c    g cg b    cg                                       eb
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                                              ENTRY      SESSION
FULL ESTIMATED COST                           2.36         5.43

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DICTIONARY FILE UPDATES:  13 SEP 2004   HIGHEST RN 744170-41-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more
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http://www.cas.org/ONLINE/DBSS/registryss.html


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h   eb c   g cg b   cg   eb

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152460-06-5/BI OR 152460-08-7/BI OR 152460-09-8/BI OR 152460-10-
1/BI OR 152460-12-3/BI OR 152460-14-5/BI OR 152460-16-7/BI OR
152460-18-9/BI OR 1535-73-5/BI OR 166306-32-7/BI OR 166306-33-8/
BI OR 166306-38-3/BI OR 179115-22-1/BI OR 2051-49-2/BI OR 21615-
34-9/BI OR 2243-83-6/BI OR 2251-50-5/BI
```

=> d scan

```
L4    75 ANSWERS    REGISTRY   COPYRIGHT 2004 ACS on STN
IN    Benzamide, 4-[(4-methyl-1-piperazinyl)methyl]-N-[4-methyl-3-[[4-(3-
      pyridinyl)-2-pyrimidinyl]amino]phenyl]- (9CI)
MF    C29 H31 N7 O
CI    COM
```
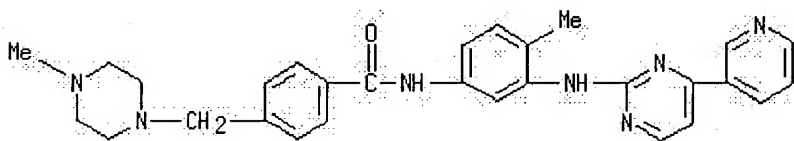

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1) 74

```
L4    75 ANSWERS    REGISTRY   COPYRIGHT 2004 ACS on STN
IN    1,3-Benzenediamine, N-[4-(4-pyridinyl)-2-pyrimidinyl]- (9CI)
MF    C15 H13 N5
```
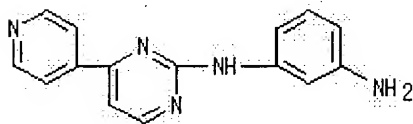

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS    REGISTRY   COPYRIGHT 2004 ACS on STN
IN    Ethanone, 1-(3-pyridinyl)- (9CI)
MF    C7 H7 N O
CI    COM
```
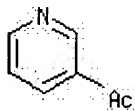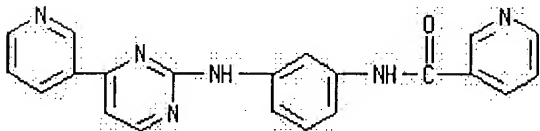

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

h   eb c   g cg b   cg   eb

L4   75 ANSWERS   REGISTRY COPYRIGHT 2004 ACS on STN
IN   2-Pyrimidinamine, 4-(3-pyridinyl)-N-[3-(1,1,2,2-tetrafluoroethoxy)phenyl]-
      (9CI)
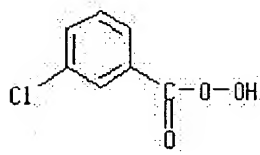MF   C17 H12 F4 N4 O
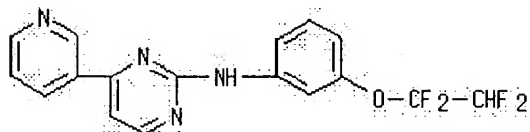
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY COPYRIGHT 2004 ACS on STN
IN   2-Pyridinecarboxamide, N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
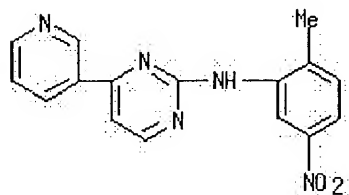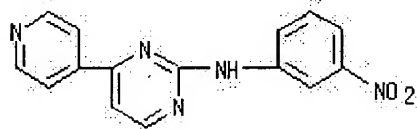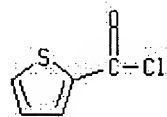   (9CI)
MF   C21 H16 N6 O
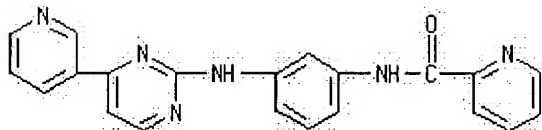
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY COPYRIGHT 2004 ACS on STN
IN   Benzoyl chloride, 4-methyl- (9CI)
MF   C8 H7 Cl O
CI   COM
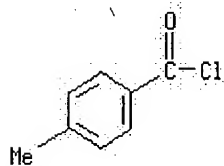
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY COPYRIGHT 2004 ACS on STN
IN   Guanidine, (2-methyl-5-nitrophenyl)-, mononitrate (9CI)
MF   C8 H10 N4 O2 . H N O3

      CM   1

h   eb c   g cg b   cg   eb

CM   2

```
      O
      ‖
O ═══ N ─ OH
```
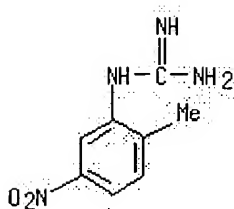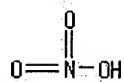
L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Pyrimidinamine, N-(3-nitrophenyl)-4-(2-pyridinyl)- (9CI)
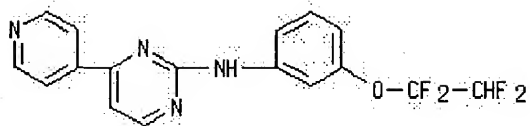MF   C15 H11 N5 O2
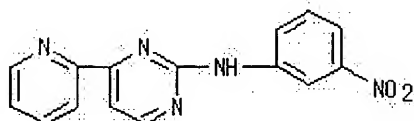
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Cyclohexanecarbonyl chloride (6CI, 7CI, 8CI, 9CI)
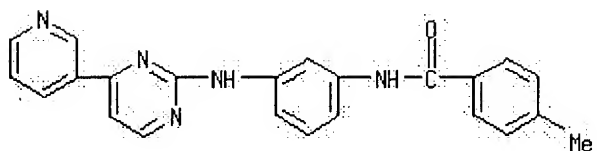MF   C7 H11 Cl O
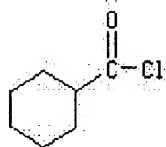
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Guanidine, [3-nitro-5-(trifluoromethyl)phenyl]-, mononitrate (9CI)
MF   C8 H7 F3 N4 O2 . H N O3

CM   1

CM   2

```
      O
      ‖
O ═══ N ─ OH
```
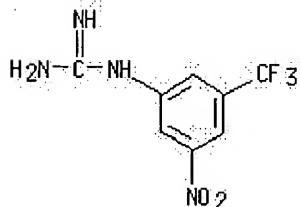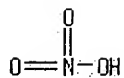
L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Cyclohexanecarboxamide, N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
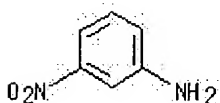   (9CI)

h   eb c   g cg b   cg   eb

MF   C22 H23 N5 O
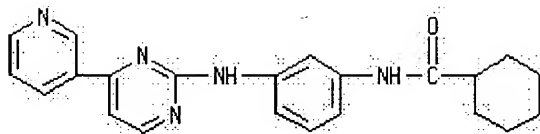
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Pyridinecarbonyl chloride (9CI)
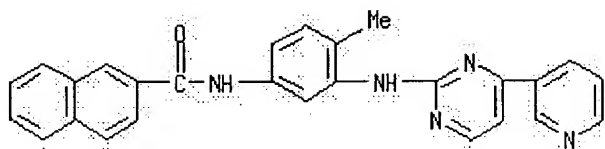MF   C6 H4 Cl N O
CI   COM
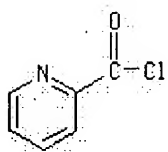
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
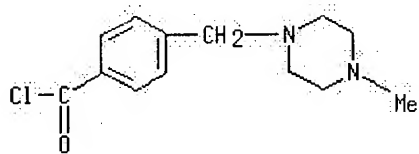IN   Benzoyl chloride (8CI, 9CI)
MF   C7 H5 Cl O
CI   COM
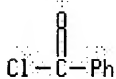
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzamide, 4-methyl-N-[4-methyl-3-[[4-(3-pyridinyl)-2-
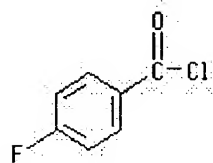   pyrimidinyl]amino]phenyl]- (9CI)
MF   C24 H21 N5 O
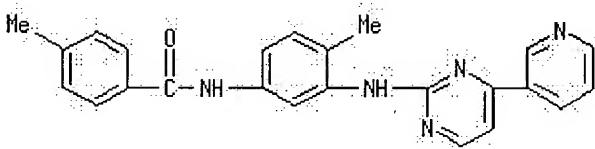
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Guanidine, (3-nitrophenyl)-, mononitrate (9CI)
MF   C7 H8 N4 O2 . H N O3

      CM   1

CM   2
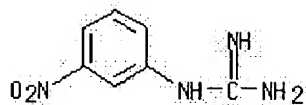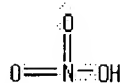
L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzenamine, 3-nitro-5-(trifluoromethyl)- (9CI)
MF   C7 H5 F3 N2 O2
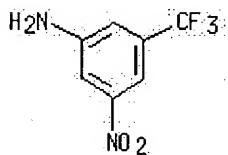
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Pyrimidinamine, N-(3-methyl-5-nitrophenyl)-4-(3-pyridinyl)- (9CI)
MF   C16 H13 N5 O2
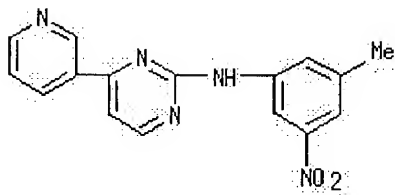
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   3-Pyridinecarboxamide, N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
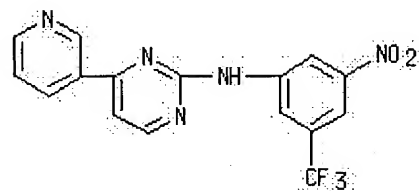   (9CI)
MF   C21 H16 N6 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzenecarboperoxoic acid, 3-chloro- (9CI)
MF   C7 H5 Cl O3
CI   COM

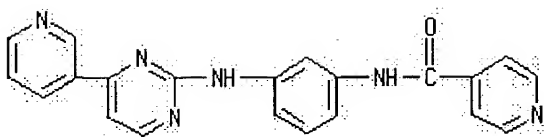h   eb c   g cg b   cg   eb

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS    REGISTRY  COPYRIGHT 2004 ACS on STN
IN    2-Pyrimidinamine, N-(2-methyl-5-nitrophenyl)-4-(3-pyridinyl)- (9CI)
MF    C16 H13 N5 O2
```


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS    REGISTRY  COPYRIGHT 2004 ACS on STN
IN    2-Pyrimidinamine, N-(3-nitrophenyl)-4-(4-pyridinyl)- (9CI)
MF    C15 H11 N5 O2
```


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS    REGISTRY  COPYRIGHT 2004 ACS on STN
IN    2-Thiophenecarbonyl chloride (6CI, 7CI, 8CI, 9CI)
MF    C5 H3 Cl O S
```


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS    REGISTRY  COPYRIGHT 2004 ACS on STN
IN    2-Pyrimidinamine, 4-(4-pyridinyl)-N-[3-(1,1,2,2-tetrafluoroethoxy)phenyl]-
      (9CI)
MF    C17 H12 F4 N4 O
```

h ,   eb c   g cg b   cg   eb
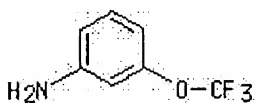
O—CF$_2$—CHF$_2$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzamide, 4-methyl-N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
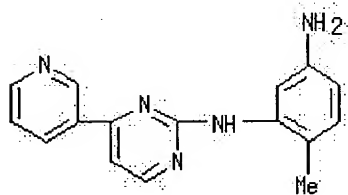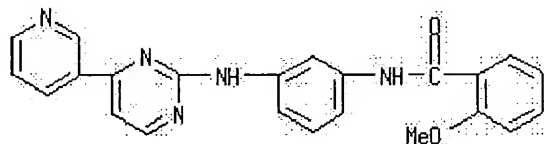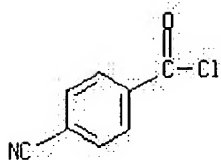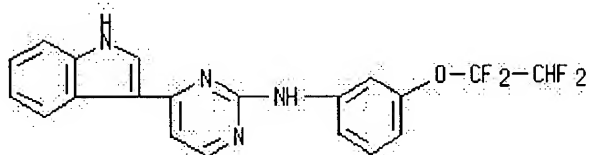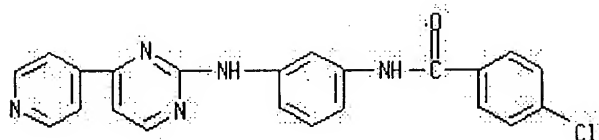   (9CI)
MF   C23 H19 N5 O

Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Propen-1-one, 3-(dimethylamino)-1-(3-pyridinyl)- (9CI)
MF   C10 H12 N2 O
CI   COM
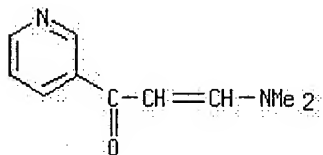
C—CH=CH—NMe$_2$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzenamine, 3-nitro- (9CI)
MF   C6 H6 N2 O2
CI   COM

O$_2$N   NH$_2$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Naphthalenecarboxamide, N-[4-methyl-3-[[4-(3-pyridinyl)-2-
      pyrimidinyl]amino]phenyl]- (9CI)
MF   C27 H21 N5 O
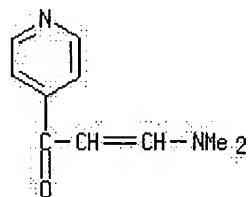
h   eb c   g cg b   cg   eb

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzoyl chloride, 4-[(4-methyl-1-piperazinyl)methyl]- (9CI)
MF   C13 H17 Cl N2 O
CI   COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzoyl chloride, 4-fluoro- (9CI)
MF   C7 H4 Cl F O
CI   COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Pyrimidinamine, N-[3-nitro-5-(trifluoromethyl)phenyl]-4-(3-pyridinyl)-
      (9CI)
MF   C16 H10 F3 N5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   4-Pyridinecarboxamide, N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
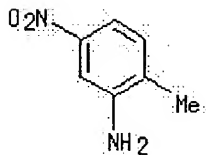   (9CI)
MF   C21 H16 N6 O

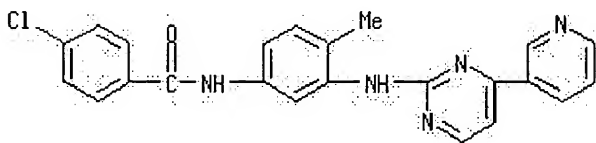h   eb c   g cg b   cg   eb

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzenamine, 3-(trifluoromethoxy)- (9CI)
MF   C7 H6 F3 N O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   1,3-Benzenediamine, 4-methyl-N3-[4-(3-pyridinyl)-2-pyrimidinyl]- (9CI)
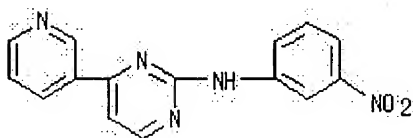MF   C16 H15 N5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzamide, 2-methoxy-N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
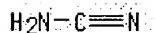   (9CI)
MF   C23 H19 N5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzoyl chloride, 4-cyano- (9CI)
MF   C8 H4 Cl N O
CI   COM

h   eb c   g cg b   cg   eb

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Pyrimidinamine, 4-(1H-indol-3-yl)-N-[3-(1,1,2,2-
     tetrafluoroethoxy)phenyl]- (9CI)
MF   C20 H14 F4 N4 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzamide, 4-chloro-N-[3-[[4-(4-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
     (9CI)
MF   C22 H16 Cl N5 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Propen-1-one, 3-(dimethylamino)-1-(4-pyridinyl)- (9CI)
MF   C10 H12 N2 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzenamine, 2-methyl-5-nitro- (9CI)
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT
MF   C7 H8 N2 O2
CI   COM

h   eb c   g cg b   cg   eb

O2N

Me

NH2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN    Benzamide, 4-chloro-N-[4-methyl-3-[[4-(3-pyridinyl)-2-
      pyrimidinyl]amino]phenyl]- (9CI)
MF    C23 H18 Cl N5 O
```
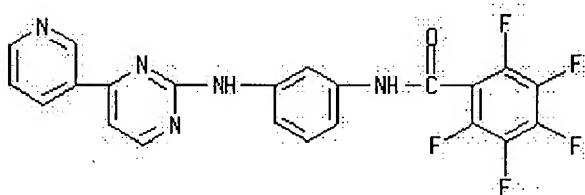
Cl

O
C—NH

Me

NH

N

N

N

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN    2-Pyrimidinamine, N-(3-nitrophenyl)-4-(3-pyridinyl)- (9CI)
MF    C15 H11 N5 O2
```
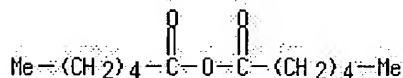
N

N

N

NH

NO2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN    Cyanamide (8CI, 9CI)
MF    C H2 N2
CI    COM
```

$H_2N—C\equiv N$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN    2-Pyrimidinamine, N-(3-nitrophenyl)-4-(1-oxido-3-pyridinyl)- (9CI)
MF    C15 H11 N5 O3
```
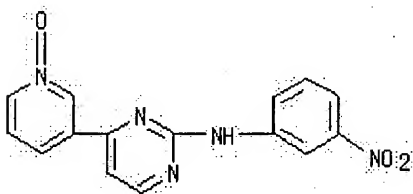
O

N

N

N

NH

NO2

h   eb c   g cg b   cg   eb

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzamide, 2,3,4,5,6-pentafluoro-N-[3-[[4-(3-pyridinyl)-2-
     pyrimidinyl]amino]phenyl]- (9CI)
MF   C22 H12 F5 N5 O
```


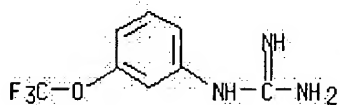**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

```
L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Hexanoic acid, anhydride (9CI)
MF   C12 H22 O3
CI   COM
```
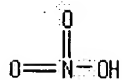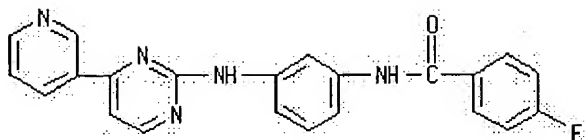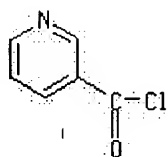

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Guanidine, [3-(trifluoromethoxy)phenyl]-, mononitrate (9CI)
MF   C8 H8 F3 N3 O . H N O3
```

```
     CM   1
```



```
     CM   2
```



```
L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzamide, 4-fluoro-N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
     (9CI)
MF   C22 H16 F N5 O
```
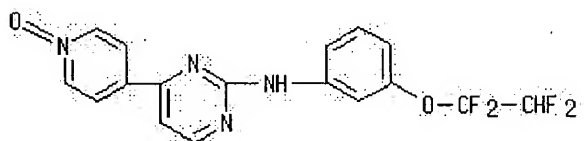
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   3-Pyridinecarbonyl chloride (9CI)
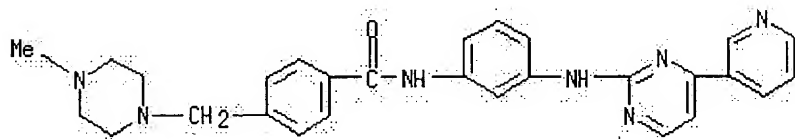MF   C6 H4 Cl N O
CI   COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Pyrimidinamine, 4-(1-oxido-4-pyridinyl)-N-[3-(1,1,2,2-
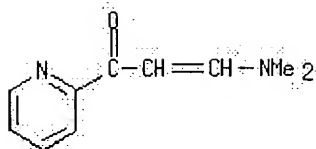   tetrafluoroethoxy)phenyl]- (9CI)
MF   C17 H12 F4 N4 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzamide, 4-[(4-methyl-1-piperazinyl)methyl]-N-[3-[[4-(3-pyridinyl)-2-
      pyrimidinyl]amino]phenyl]- (9CI)
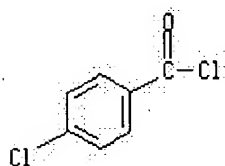MF   C28 H29 N7 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Propen-1-one, 3-(dimethylamino)-1-(2-pyridinyl)- (9CI)
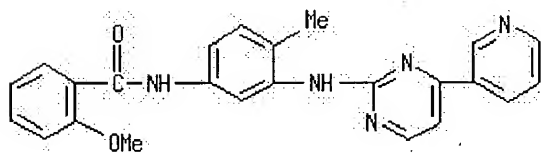MF   C10 H12 N2 O

h   eb c   g cg b   cg   eb

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4   75 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN   Benzoyl chloride, 4-chloro- (9CI)
MF   C7 H4 Cl2 O
CI   COM
```
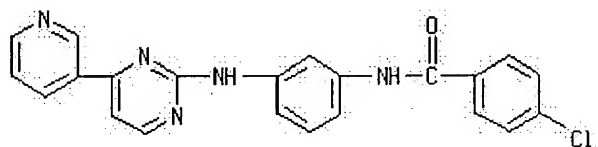

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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L4   75 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN   Benzamide, 2-methoxy-N-[4-methyl-3-[[4-(3-pyridinyl)-2-
     pyrimidinyl]amino]phenyl]- (9CI)
MF   C24 H21 N5 O2
```
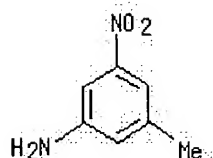

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4   75 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN   Benzamide, 4-chloro-N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
     (9CI)
MF   C22 H16 Cl N5 O
```
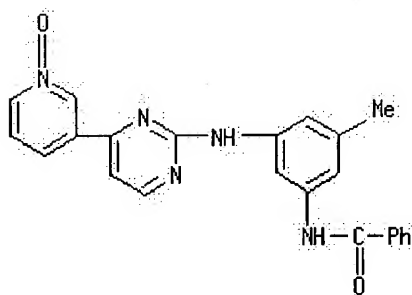

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4   75 ANSWERS   REGISTRY  COPYRIGHT 2004 ACS on STN
IN   Benzenamine, 3-methyl-5-nitro- (9CI)
MF   C7 H8 N2 O2
```

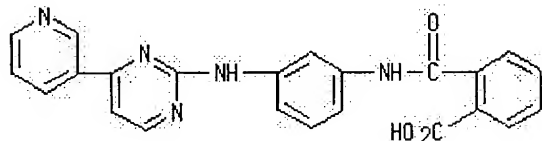h   eb c   g cg b   cg   eb

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzamide, N-[3-methyl-5-[[4-(1-oxido-3-pyridinyl)-2-
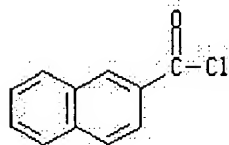   pyrimidinyl]amino]phenyl]- (9CI)
MF   C23 H19 N5 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzoic acid, 2-[[[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]amino]ca
      rbonyl]- (9CI)
MF   C23 H17 N5 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Naphthalenecarbonyl chloride (9CI)
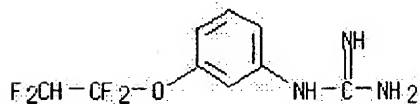MF   C11 H7 Cl O
CI   COM
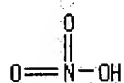

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN

h   eb c   g cg b   cg   eb

IN   Guanidine, [3-(1,1,2,2-tetrafluoroethoxy)phenyl]-, mononitrate (9CI)
MF   C9 H9 F4 N3 O . H N O3

    CM   1

F 2CH — CF 2 — O — [phenyl] — NH — C(=NH) — NH 2
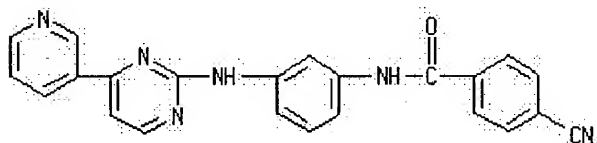
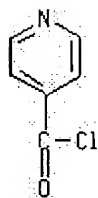   CM   2

O = N — OH (with O above N)

L4   75 ANSWERS   REGISTRY COPYRIGHT 2004 ACS on STN
IN   Benzamide, 4-cyano-N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
    (9CI)
MF   C23 H16 N6 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY COPYRIGHT 2004 ACS on STN
IN   4-Pyridinecarbonyl chloride (9CI)
MF   C6 H4 Cl N O
CI   COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY COPYRIGHT 2004 ACS on STN
IN   Benzamide, N-[3-methyl-5-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
    (9CI)
MF   C23 H19 N5 O

h   eb c   g cg b   cg   eb

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzamide, N-[4-methyl-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
     (9CI)
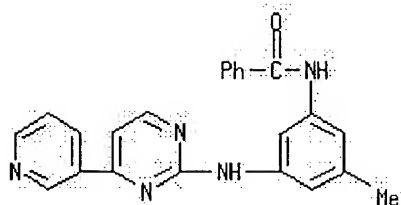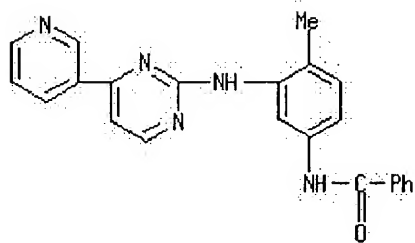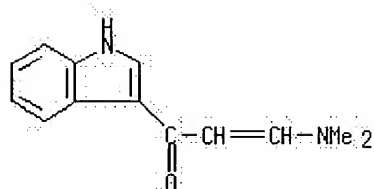MF   C23 H19 N5 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Propen-1-one, 3-(dimethylamino)-1-(1H-indol-3-yl)- (9CI)
MF   C13 H14 N2 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Methanamine, N-methyl- (9CI)
MF   C2 H7 N
CI   COM

H3C—NH—CH3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Pyrimidinamine, 4-(3-pyridinyl)-N-[3-(trifluoromethoxy)phenyl]- (9CI)
MF   C16 H11 F3 N4 O
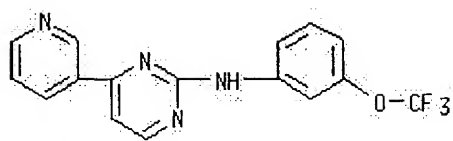
h   eb c   g cg b   cg   eb

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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L4    75 ANSWERS    REGISTRY   COPYRIGHT 2004 ACS on STN
IN    Benzamide, N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]- (9CI)
MF    C22 H17 N5 O
```
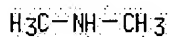

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS    REGISTRY   COPYRIGHT 2004 ACS on STN
IN    Benzenamine, 3-(1,1,2,2-tetrafluoroethoxy)- (9CI)
MF    C8 H7 F4 N O
```


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L4    75 ANSWERS    REGISTRY   COPYRIGHT 2004 ACS on STN
IN    1,3-Benzenediamine, N-[4-(3-pyridinyl)-2-pyrimidinyl]- (9CI)
MF    C15 H13 N5
CI    COM
```


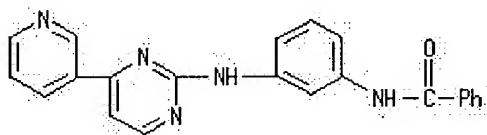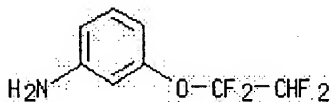**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

```
L4    75 ANSWERS    REGISTRY   COPYRIGHT 2004 ACS on STN
IN    Hexanamide, N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]- (9CI)
MF    C21 H23 N5 O
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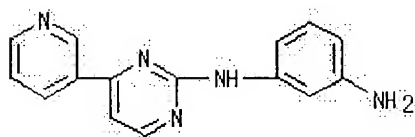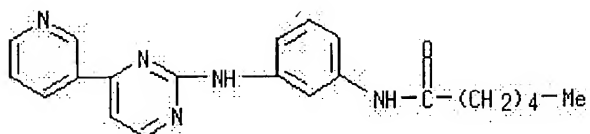
h   eb c   g cg b   cg   eb

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Benzoyl chloride, pentafluoro- (6CI, 7CI, 8CI, 9CI)
MF   C7 Cl F5 O
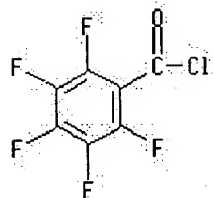
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   Guanidine, (3-methyl-5-nitrophenyl)-, mononitrate (9CI)
MF   C8 H10 N4 O2 . H N O3

    CM   1

    CM   2
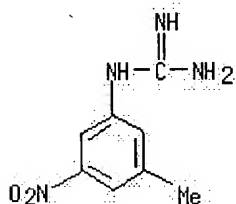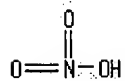
L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   2-Thiophenecarboxamide, N-[3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]-
      (9CI)
MF   C20 H15 N5 O S
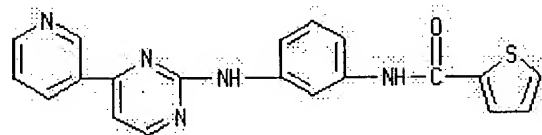
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN

h   eb c   g cg b   cg   eb

IN   Benzoyl chloride, 2-methoxy- (9CI)
MF   C8 H7 Cl O2
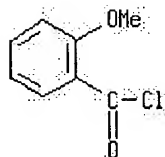
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4   75 ANSWERS   REGISTRY   COPYRIGHT 2004 ACS on STN
IN   1,3-Isobenzofurandione (9CI)
MF   C8 H4 O3
CI   COM
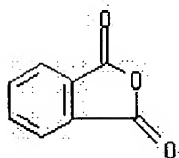
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=>

h   eb c   g cg b   cg   eb

* * * * * * * * *   Welcome to STN International   * * * * * * * * * *

NEWS 1   Web Page URLs for STN Seminar Schedule - N. America
NEWS 2   "Ask CAS" for self-help around the clock
NEWS 3   May 12 EXTEND option available in structure searching
NEWS 4   May 12 Polymer links for the POLYLINK command completed in REGISTRY
NEWS 5   May 27 New UPM (Update Code Maximum) field for more efficient patent
                   SDIs in CAplus
NEWS 6   May 27 CAplus super roles and document types searchable in REGISTRY
NEWS 7   Jun 28 Additional enzyme-catalyzed reactions added to CASREACT
NEWS 8   Jun 28 ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG,
                   and WATER from CSA now available on STN(R)
NEWS 9   Jul 12 BEILSTEIN enhanced with new display and select options,
                   resulting in a closer connection to BABS
NEWS 10   Jul 30 BEILSTEIN on STN workshop to be held August 24 in conjunction
                   with the 228th ACS National Meeting
NEWS 11   AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display
                   fields
NEWS 12   AUG 02 CAplus and CA patent records enhanced with European and Japan
                   Patent Office Classifications
NEWS 13   AUG 02 STN User Update to be held August 22 in conjunction with the
                   228th ACS National Meeting
NEWS 14   AUG 02 The Analysis Edition of STN Express with Discover!
                   (Version 7.01 for Windows) now available
NEWS 15   AUG 04 Pricing for the Save Answers for SciFinder Wizard within
                   STN Express with Discover! will change September 1, 2004
NEWS 16   AUG 27 BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 17   AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal
                   status data from INPADOC
NEWS 18   SEP 01 INPADOC: New family current-awareness alert (SDI) available
NEWS 19   SEP 01 New pricing for the Save Answers for SciFinder Wizard within
                   STN Express with Discover!
NEWS 20   SEP 01 New display format, 'HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS 21   SEP 14 STN Patent Forum to be held October 13, 2004, in Iselin, NJ

NEWS EXPRESS   JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT
                MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
                AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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NEWS INTER   General Internet Information
NEWS LOGIN   Welcome Banner and News Items
NEWS PHONE   Direct Dial and Telecommunication Network Access to STN
NEWS WWW   CAS World Wide Web Site (general information)

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specific topic.

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   * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 19:52:17 ON 14 SEP 2004

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                              ENTRY   SESSION

h   eb c   g cg b   cg   eb

FULL ESTIMATED COST   0.21   0.21

FILE 'REGISTRY' ENTERED AT 19:52:22 ON 14 SEP 2004
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STRUCTURE FILE UPDATES: 13 SEP 2004   HIGHEST RN 744170-41-0
DICTIONARY FILE UPDATES: 13 SEP 2004   HIGHEST RN 744170-41-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

    Please note that search-term pricing does apply when
    conducting SmartSELECT searches.

Crossover limits have been increased.   See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
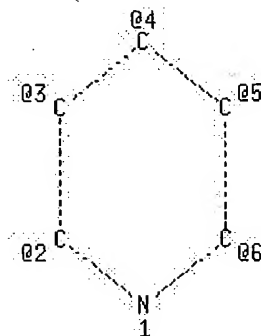http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR
 0 22 S 23

Page 1-A

h   eb c   g cg b   cg   eb
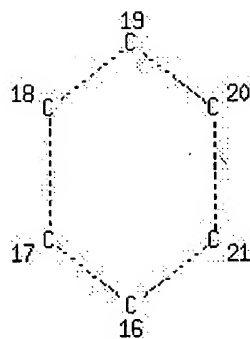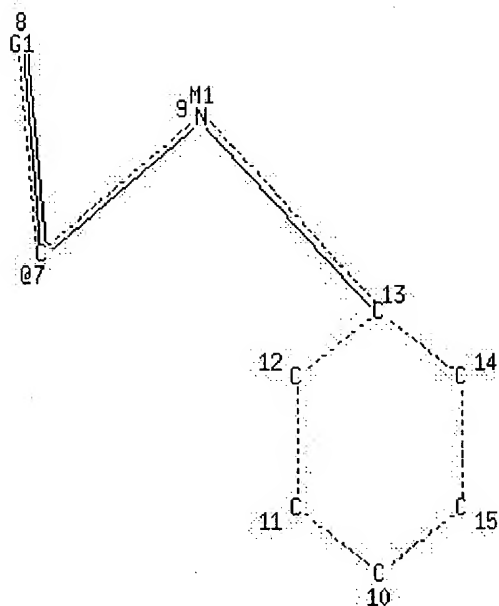
Page 1-B
VAR G1=22/23
VPA 7-2/3/4/5/6 S
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NSPEC   IS R   AT   1
NSPEC   IS R   AT   2
NSPEC   IS R   AT   3
NSPEC   IS R   AT   4
NSPEC   IS R   AT   5
NSPEC   IS R   AT   6
NSPEC   IS C   AT   7
NSPEC   IS C   AT   8
NSPEC   IS C   AT   9
NSPEC   IS R   AT   10
NSPEC   IS R   AT   11
NSPEC   IS R   AT   12
NSPEC   IS R   AT   13
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NSPEC   IS R   AT   21
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MLEVEL   IS CLASS   AT   7   9 22 23
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS   23

STEREO ATTRIBUTES: NONE

=> s 11
SAMPLE SEARCH INITIATED 19:54:14 FILE 'REGISTRY'

h   eb c   g cg b   cg   eb

SAMPLE SCREEN SEARCH COMPLETED -   4616 TO ITERATE

 21.7% PROCESSED   1000 ITERATIONS   50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **COMPLETE**
                         BATCH   **COMPLETE**
PROJECTED ITERATIONS: 88247 TO   96393
PROJECTED ANSWERS: 6829 TO   9233

L2   50 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 19:54:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 90823 TO ITERATE

100.0% PROCESSED   90823 ITERATIONS   7359 ANSWERS
SEARCH TIME: 00.00.01

L3   7359 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                ENTRY   SESSION

FULL ESTIMATED COST   156.68   156.89

FILE 'HCAPLUS' ENTERED AT 19:54:29 ON 14 SEP 2004
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FILE COVERS 1907 - 14 Sep 2004 VOL 141 ISS 12
FILE LAST UPDATED: 13 Sep 2004 (20040913/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s l3/thu
         1356 L3
       619171 THU/RL
L4   314 L3/THU
             (L3 (L) THU/RL)

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL

h   eb c   g cg b   cg   eb

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                                              ENTRY     SESSION
FULL ESTIMATED COST                           2.36       159.25

FILE 'REGISTRY' ENTERED AT 19:54:36 ON 14 SEP 2004
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STRUCTURE FILE UPDATES:   13 SEP 2004  HIGHEST RN 744170-41-0
DICTIONARY FILE UPDATES:  13 SEP 2004  HIGHEST RN 744170-41-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L5        STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5                STR

=> s l5
SAMPLE SEARCH INITIATED 19:56:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     45 TO ITERATE


100.0% PROCESSED      45 ITERATIONS                      0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE  **COMPLETE**
                         BATCH   **COMPLETE**
PROJECTED ITERATIONS:      498 TO      1302
PROJECTED ANSWERS:           0 TO         0

L6           0 SEA SSS SAM L5

=> s l5 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 19:56:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    896 TO ITERATE


100.0% PROCESSED      896 ITERATIONS                     0 ANSWERS
SEARCH TIME: 00.00.01

L7           0 SEA SSS FUL L5

=>
L8        STRUCTURE UPLOADED



  h       eb c    g cg  b    cg                            eb
```

```
=> d l8
L8  HAS NO ANSWERS
L8                STR

=> s l8
SAMPLE SEARCH INITIATED 19:58:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      2 TO ITERATE

100.0% PROCESSED      2 ITERATIONS                         0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           2 TO       124
PROJECTED ANSWERS:              0 TO         0

L9            0 SEA SSS SAM L8

=> s l8 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 19:58:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     63 TO ITERATE

100.0% PROCESSED     63 ITERATIONS                         0 ANSWERS
SEARCH TIME: 00.00.01

L10           0 SEA SSS FUL L8

=>
L11      STRUCTURE UPLOADED

=> d l11
L11 HAS NO ANSWERS
L11              STR

=> s l11
SAMPLE SEARCH INITIATED 20:00:51 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      0 TO ITERATE

100.0% PROCESSED      0 ITERATIONS                         0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           0 TO         0
PROJECTED ANSWERS:              0 TO         0

L12           0 SEA SSS SAM L11

=> s l11
SAMPLE SEARCH INITIATED 20:00:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      0 TO ITERATE

100.0% PROCESSED      0 ITERATIONS                         0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
```

h   eb c   g cg b   cg   eb

```
PROJECTED ITERATIONS:              0 TO          0
PROJECTED ANSWERS:                 0 TO          0


L13              0 SEA SSS SAM L11


=> s l11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:00:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     23 TO ITERATE


100.0% PROCESSED       23 ITERATIONS                       0 ANSWERS
SEARCH TIME: 00.00.01


L14              0 SEA SSS FUL L11


=>
L15      STRUCTURE UPLOADED


=> d l15
L15 HAS NO ANSWERS
L15              STR


=> s l15
SAMPLE SEARCH INITIATED 20:04:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     18 TO ITERATE


100.0% PROCESSED       18 ITERATIONS                       0 ANSWERS
SEARCH TIME: 00.00.01


FULL FILE PROJECTIONS:   ONLINE   **COMPLETE**
                         BATCH    **COMPLETE**
PROJECTED ITERATIONS:            106 TO         614
PROJECTED ANSWERS:                 0 TO          0


L16              0 SEA SSS SAM L15


=> s l15 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:04:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    449 TO ITERATE


100.0% PROCESSED      449 ITERATIONS                       0 ANSWERS
SEARCH TIME: 00.00.01


L17              0 SEA SSS FUL L15


=>
L18      STRUCTURE UPLOADED


=> d l18
L18 HAS NO ANSWERS
L18              STR


=> s l18
SAMPLE SEARCH INITIATED 20:06:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      0 TO ITERATE


100.0% PROCESSED        0 ITERATIONS                       0 ANSWERS
```

h   eb c   g cg b   cg   eb

```
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   **COMPLETE**
                         BATCH    **COMPLETE**
PROJECTED ITERATIONS:              0 TO          0
PROJECTED ANSWERS:                 0 TO          0


L19            0 SEA SSS SAM L18


=> s l18 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:06:54 FILE 'REGISTRY'
FULL 'SCREEN SEARCH COMPLETED -    14 TO ITERATE

100.0% PROCESSED      14 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.01

L20            0 SEA SSS FUL L18

=>
```

h   eb c   g cg b   cg   eb
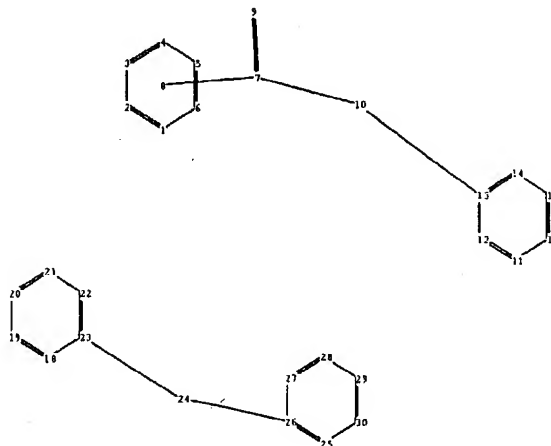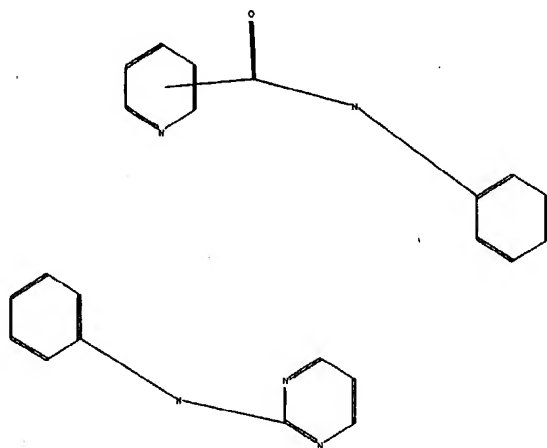
chain nodes :
    7 9 10 24
ring nodes :
    1 2 3 4 5 6 11 12 13 14 15 16 18 19 20 21 22 23 25 26 27 28 29 30
chain bonds :
    7-9 7-10 10-13 23-24 24-26
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 18-19 18-23
    19-20 20-21 21-22 22-23 25-26 25-30 26-27 27-28 28-29 29-30
exact/norm bonds :
   7-9 7-10 10-13 23-24 24-26
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 18-19 18-23
    19-20 20-21 21-22 22-23 25-26 25-30 26-27 27-28 28-29 29-30
isolated ring systems :
    containing 1 : 11 : 18 : 25 :

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
    11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:Atom 21:Atom
    22:Atom 23:Atom 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
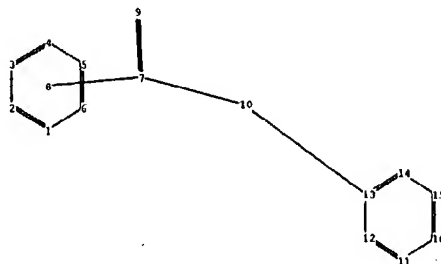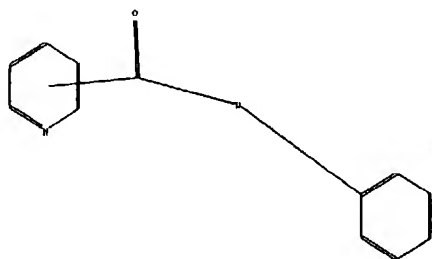
chain nodes :
    7 9 10
ring nodes :
    1 2 3 4 5 6 11 12 13 14 15 16
chain bonds :
    7-9 7-10 10-13
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16
exact/norm bonds :
    7-9 7-10 10-13
normalized bonds :
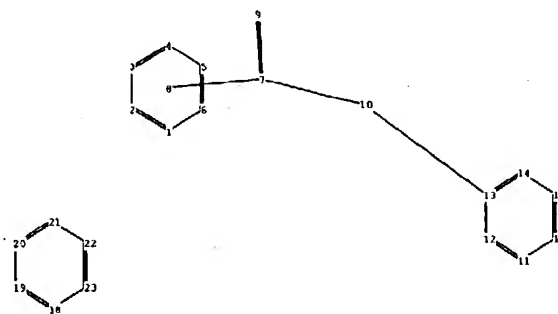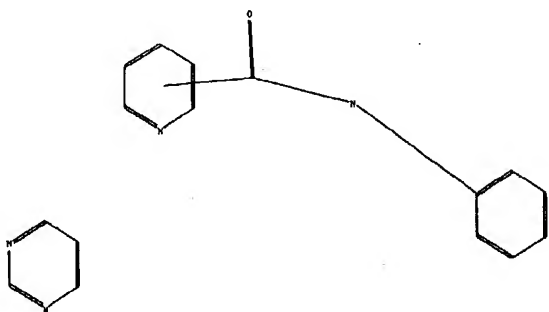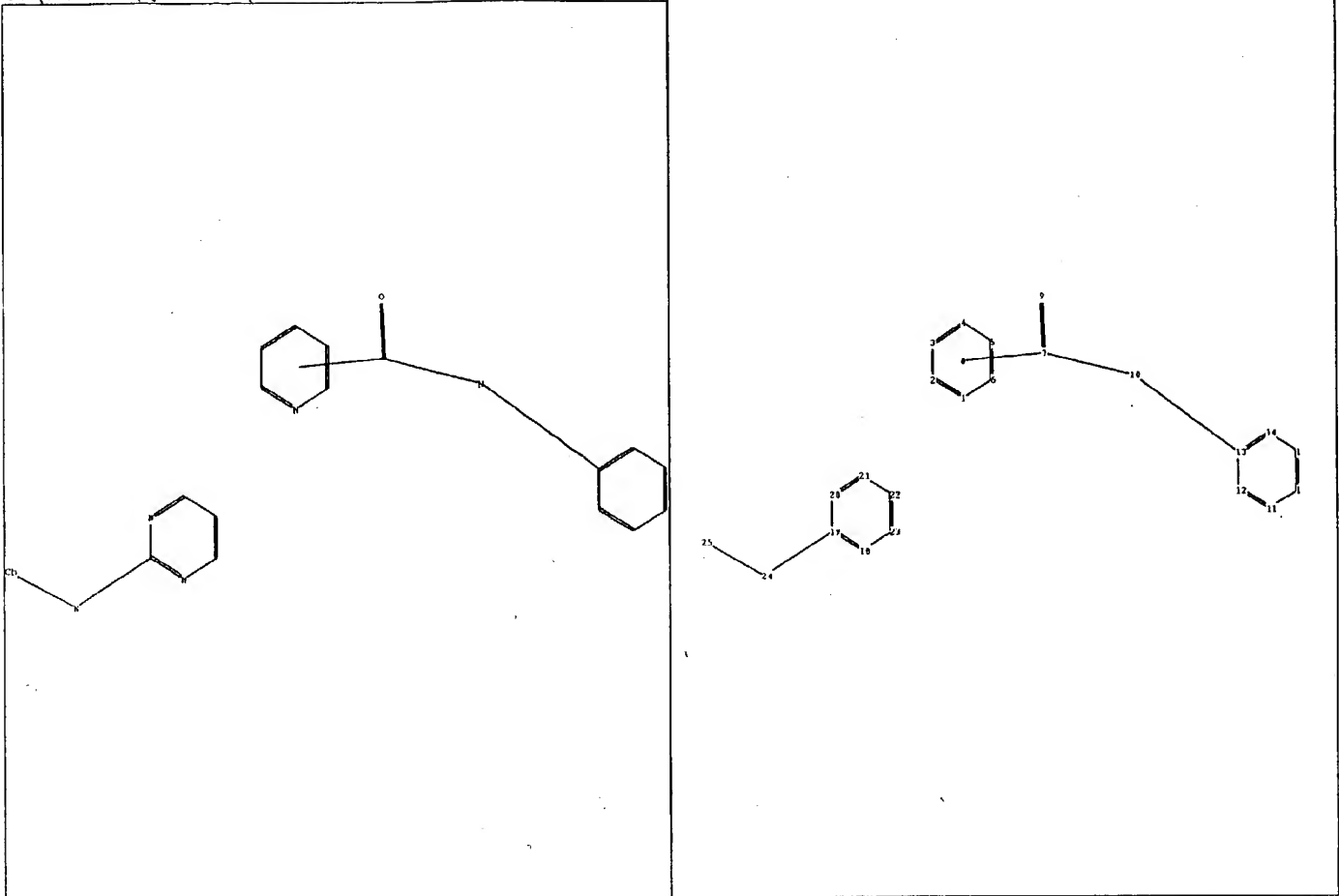   1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16
isolated ring systems :
    containing 1 : 11 :

match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
    11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom

chain nodes :
    7 9 10
ring nodes :
    1   2   3   4   5   6   11   12   13   14   15   16 18   19   20   21   22   23
chain bonds :
    7-9   7-10   10-13
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   11-12   11-16   12-13   13-14   14-15   15-16   18-19   18-23
    19-20   20-21   21-22   22-23
exact/norm bonds :
    7-9   7-10   10-13
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   11-12   11-16   12-13   13-14   14-15   15-16   18-19   18-23
    19-20   20-21   21-22   22-23
isolated ring systems :
    containing 1 : 11 : 18 :

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS   10:CLASS
    11:Atom   12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   18:Atom   19:Atom   20:Atom   21:Atom
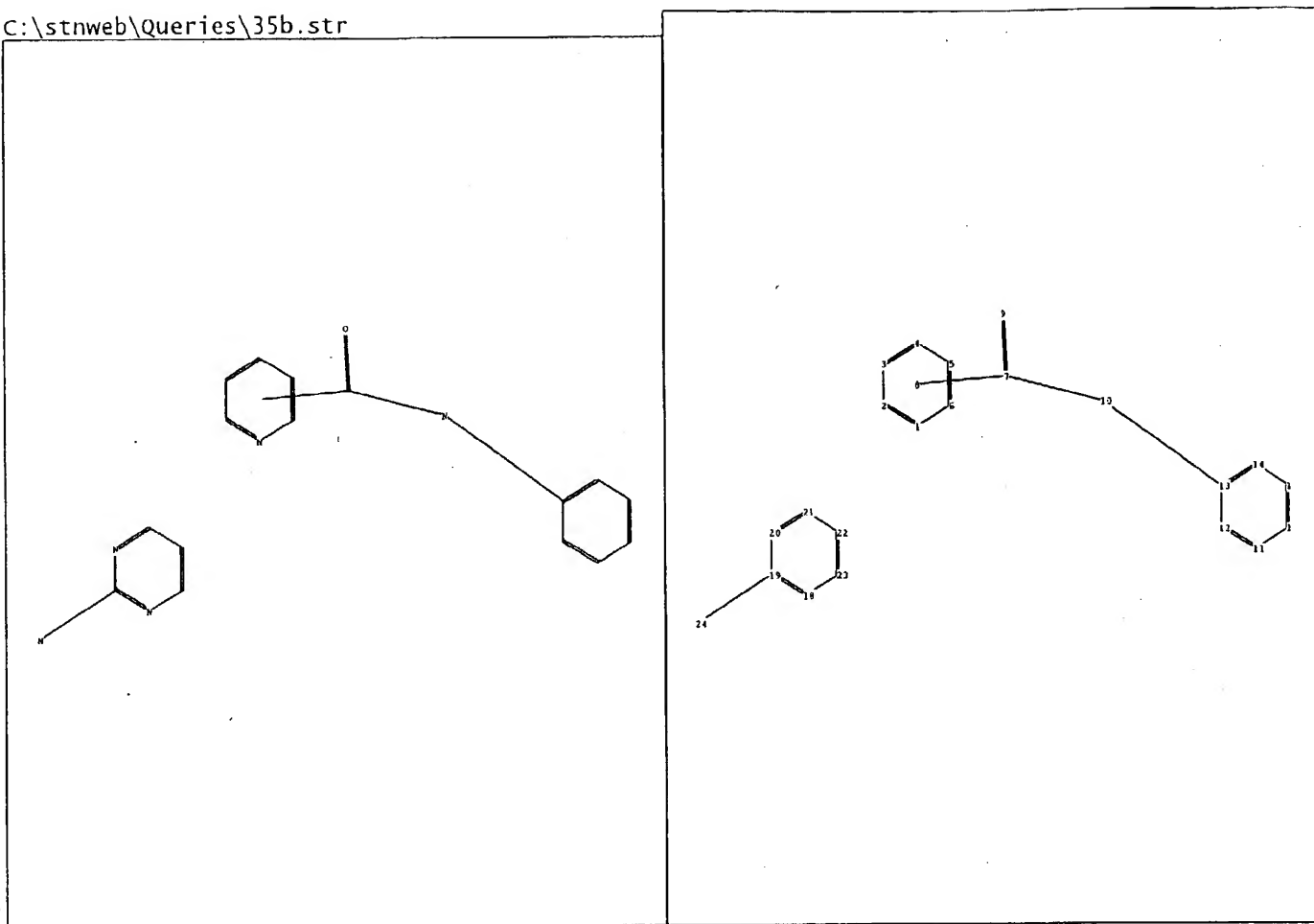   22:Atom   23:Atom

chain nodes :
    7 9 10 24 25
ring nodes :
    1 2 3 4 5 6 11 12 13 14 15 16 18 19 20 21 22 23
chain bonds :
    7-9 7-10 10-13 19-24 24-25
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 18-19 18-23
    19-20 20-21 21-22 22-23
exact/norm bonds :
    7-9 7-10 10-13 19-24
exact bonds :
    24-25
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 18-19 18-23
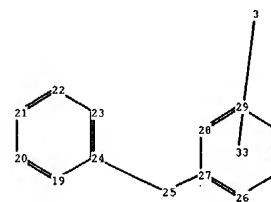   19-20 20-21 21-22 22-23
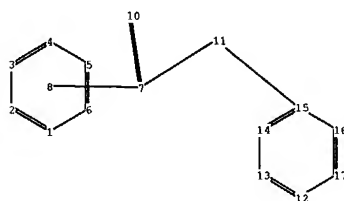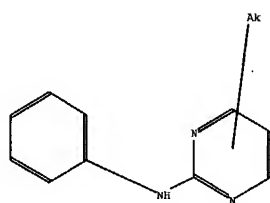isolated ring systems :
    containing 1 : 11 : 18 :

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
    11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:Atom 21:Atom
    22:Atom 23:Atom 24:CLASS 25:Atom

chain nodes :
    7 9 10 24
ring nodes :
    1 2 3 4 5 6 11 12 13 14 15 16 18 19 20 21 22 23
chain bonds :
    7-9 7-10 10-13 19-24
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 18-19 18-23
    19-20 20-21 21-22 22-23
exact/norm bonds :
    7-9 7-10 10-13 19-24
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 18-19 18-23
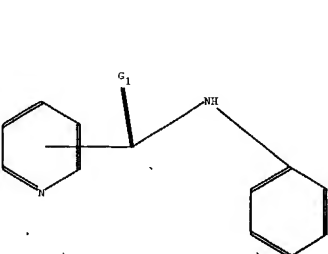   19-20 20-21 21-22 22-23
isolated ring systems :
    containing 1 : 11 : 18 :

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
    11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:Atom 21:Atom
    22:Atom 23:Atom 24:CLASS

hain nodes :
    7   10   11   25   32
ing nodes :
    1   2   3   4   5   6   12   13   14   15   16   17   19   20   21   22   23   24   26   27   28   29   30   31
hain bonds :
    7-10   7-11   11-15   24-25   25-27
ing bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   12-13   12-17   13-14   14-15   15-16   16-17   19-20   19-24
    20-21   21-22   22-23   23-24   26-27   26-31   27-28   28-29   29-30   30-31
xact/norm bonds :
    7-10   7-11   11-15   24-25   25-27
ormalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   12-13   12-17   13-14   14-15   15-16   16-17   19-20   19-24
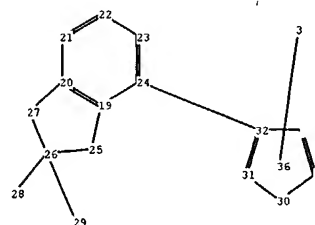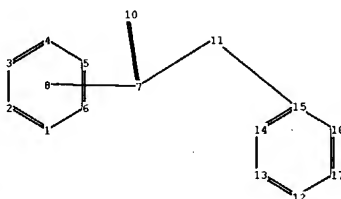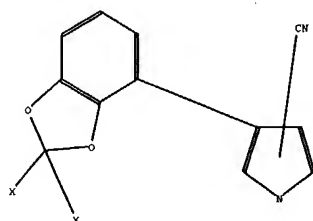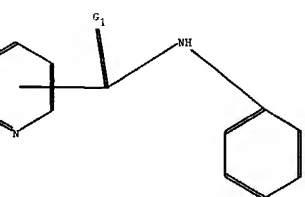   20-21   21-22   22-23   23-24   26-27   26-31   27-28   28-29   29-30   30-31
solated ring systems :
    containing 1 : 12 : 19 :

1:O,S

atch level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   10:CLASS   11:CLASS
    12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   19:Atom   20:Atom   21:Atom   22:Atom
    23:Atom   24:Atom   25:CLASS   26:Atom   27:Atom   28:Atom   29:Atom   30:Atom   31:Atom
    32:CLASS   33:CLASS

in nodes :
 7   10   11   28   29   35
g nodes :
 1   2   3   4   5   6   12   13   14   15   16   17   19   20   21   22   23   24   25   26   27   30   31   32
 33   34
in bonds :
 7-10   7-11   11-15   24-32   26-28   26-29
g bonds :
 1-2   1-6   2-3   3-4   4-5   5-6   12-13   12-17   13-14   14-15   15-16   16-17   19-20   19-24
 19-25   20-21   20-27   21-22   22-23   23-24   25-26   26-27   30-31   30-34   31-32   32-33   33-34
ct/norm bonds :
 7-10   7-11   11-15   30-31   30-34   31-32   32-33   33-34
ct bonds :
 19-25   20-27   24-32   25-26   26-27   26-28   26-29
malized bonds :
 1-2   1-6   2-3   3-4   4-5   5-6   12-13   12-17   13-14   14-15   15-16   16-17   19-20   19-24
 20-21   21-22   22-23   23-24
lated ring systems :
 containing 1 : 12 : 19 :


o,s

ch level :
 1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   10:CLASS   11:CLASS
 12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   19:Atom   20:Atom   21:Atom   22:Atom
 23:Atom   24:Atom   25:Atom   26:Atom   27:Atom   28:CLASS   29:CLASS   30:Atom   31:Atom
 32:Atom   33:Atom   34:Atom   35:CLASS   36:CLASS
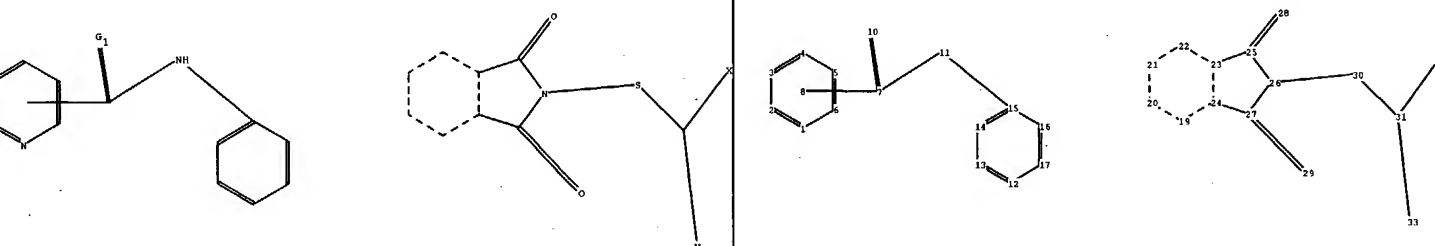
hain nodes :
    7   10   11   28   29   30   31   32   33
ing nodes :
    1   2   3   4   5   6   12   13   14   15   16   17   19   20   21   22   23   24   25   26   27
hain bonds :
    7-10   7-11   11-15   25-28   26-30   27-29   30-31   31-32   31-33
ing bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   12-13   12-17   13-14   14-15   15-16   16-17   19-20   19-24
    20-21   21-22   22-23   23-24   23-25   24-27   25-26   26-27
xact/norm bonds :
    7-10   7-11   11-15   19-20   19-24   20-21   21-22   22-23   23-24   25-26   25-28   26-27   26-30
    27-29   30-31
xact bonds :
    23-25   24-27   31-32   31-33
ormalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   12-13   12-17   13-14   14-15   15-16   16-17
solated ring systems :
    containing 1 : 12 : 19 :

1:o,s

atch level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   10:CLASS   11:CLASS
    12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   19:Atom   20:Atom   21:Atom   22:Atom
    23:Atom   24:Atom   25:Atom   26:Atom   27:Atom   28:CLASS   29:CLASS   30:CLASS   31:CLASS
    32:CLASS   33:CLASS
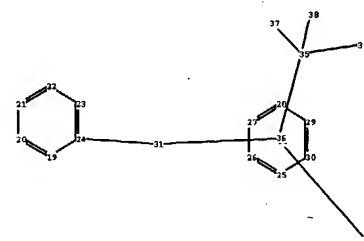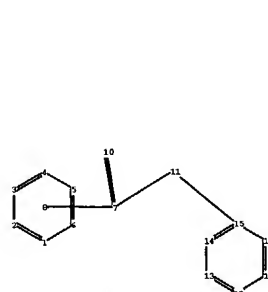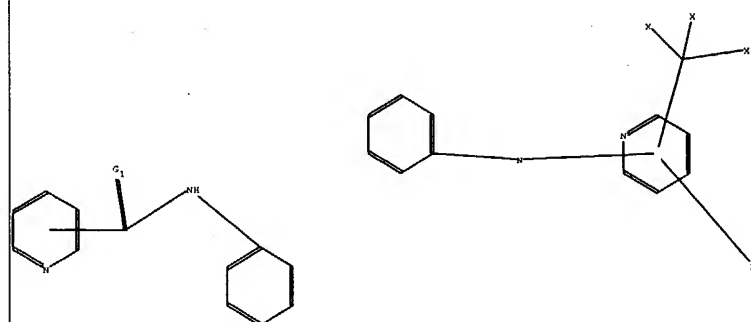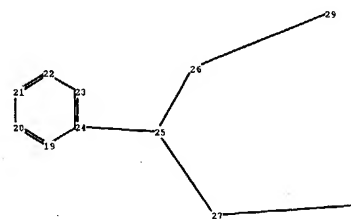
chain nodes :
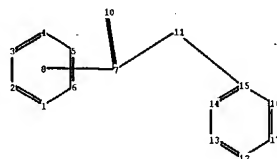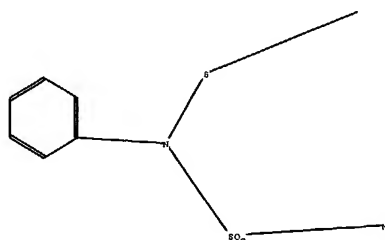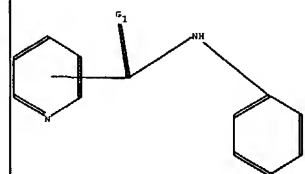   7   10   11   31   33   35   37   38   39
ring nodes :
    1   2   3   4   5   6   12   13   14   15   16   17   19   20   21   22   23   24   25   26   27   28   29   30
chain bonds :
    7-10   7-11   11-15   24-31   35-39   35-38   35-37
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   12-13   12-17   13-14   14-15   15-16   16-17   19-20   19-24
    20-21   21-22   22-23   23-24   25-26   25-30   26-27   27-28   28-29   29-30
exact/norm bonds :
    7-10   7-11   11-15   24-31
exact bonds :
    35-39   35-38   35-37
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   12-13   12-17   13-14   14-15   15-16   16-17   19-20   19-24
    20-21   21-22   22-23   23-24   25-26   25-30   26-27   27-28   28-29   29-30
isolated ring systems :
    containing 1 : 12 : 19 :

G1:O,S

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS
    12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:Atom 20:Atom 21:Atom 22:Atom
    23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS
    32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS

chain nodes :
    7   10   11   25   26   27   28   29
ring nodes :
    1   2   3   4   5   6   12   13   14   15   16   17   19   20   21   22   23   24
chain bonds :
    7-10   7-11   11-15   24-25   25-26   25-27   26-29   27-28
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   12-13   12-17   13-14   14-15   15-16   16-17   19-20   19-24
    20-21   21-22   22-23   23-24
exact/norm bonds :
    7-10   7-11   11-15   24-25   25-26   25-27   26-29   27-28
normalized bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   12-13   12-17   13-14   14-15   15-16   16-17   19-20   19-24
    20-21   21-22   22-23   23-24
isolated ring systems :
    containing 1 : 12 : 19 :

G1:O,S

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   10:CLASS   11:CLASS
    12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   19:Atom   20:Atom   21:Atom   22:Atom
    23:Atom   24:Atom   25:CLASS   26:CLASS   27:CLASS   28:CLASS   29:CLASS